BIOGRAPHICAL SKETCH

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NAME: Bruce C Gibb

eRA COMMONS USER NAME (credential, e.g., agency login): bcgibb

POSITION TITLE: Professor of Chemistry

EDUCATION/TRAINING

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	Completion Date MM/YYYY	FIELD OF STUDY
Robert Gordon's University, Aberdeen, UK	B.Sc.	06/1987	Physical Sciences
Robert Gordon's University, Aberdeen, UK	Ph.D.	06/1992	Organic Chemistry
University of British Columbia, Vancouver	Postdoc	10/1994	Supramolecular Chem.
New York University, New York	Postdoc	07/1996	Bioorganic Chemistry

A. Personal Statement

The current application builds on our five-year collaboration with Profs. David Mobley (UC Irvine) and Michael Gilson (UC San Diego), which in turn stems from my 20 years of independent research on aqueous supramolecular chemistry. Our work with Mobley and Gilson has centered round the Statistical Assessment of the Modeling of Proteins and Ligands (SAMPL) exercise (OpenEye Scientific).[1,2] In this collaboration our group synthesizes host and guest molecules and then utilizes Isothermal Titration Calorimetry (ITC) to determine the thermodynamics of host-guest complexation. Our data is sealed until the group of computational chemists marshaled by Mobley and Gilson has, *a priori*, calculated the thermodynamics of the different binding events. Whilst this exercise has proven to be invaluable for computational chemists to test the predictive powers of their different approaches, the scrutiny our results receives also ensures exceedingly high standards of data collection within my own group; a fact that I consider essential to student training as research scientists.

The SAMPL exercise dove-tails with our ongoing research into a family of hosts we use[3] to probe the complex relationship between the Hydrophobic effect and solute shape,[4] and how salts influence aqueous solutions, i.e., the Hofmeister effect. Additionally, as is described below, we use our understanding of these phenomena to study molecular compartmentalization within yocto liter spaces, and how this can be used to bring about novel purification protocols and unusual chemical reactions.

1. Sullivan M. R., Sokkalingam P., Nguyen T., Donahue J. P., Gibb B. C. Binding of carboxylate and trimethylammonium salts to octa-acid and TEMOA deep-cavity cavitands. J. Comput. Aided Mol. Des., 2016, SAMPL5 Special Issue. doi: 10.1007/s10822-016-9925-0. PubMed PMID: 27432339.
2. Gibb C. L. D., Gibb B. C. *Binding of cyclic carboxylates to octa-acid deep-cavity cavitand*. J. Comput. Aided Mol. Des., **2014**, *28*(4), 319-25. doi: 10.1007/s10822-013-9690-2. PubMed PMID: 24218290; PubMed Central PMCID: PMC4018434.
3. Jordan J. H., Gibb B. C. *Molecular containers assembled through the hydrophobic effect*. Chem Soc Rev, **2015**, *44*(2), 547-85. doi: 10.1039/c4cs00191e. PubMed PMID: 25088697.
4. Hillyer M. B., Gibb B. C. *Molecular Shape and the Hydrophobic Effect*. Annu. Rev. Phys. Chem., **2016**, *67*, 307-29. doi: 10.1146/annurev-physchem-040215-112316. PubMed PMID: 27215816.

B. Positions and Honors

Positions:

1996-2002	Assistant Professor, Department of Chemistry, Univ. of New Orleans (UNO)
2002-2005	Associate Professor, Department of Chemistry, UNO, LA
2005-2008	Professor of Chemistry, Department of Chemistry, UNO, LA
2008-2011	University Research Professor of Chemistry, Department of Chemistry, UNO, LA
2012-	Professor of Chemistry, Tulane University, LA

Other experiences and professional memberships:

1996-	Member, American Chemical Society, American Association for the Advancement of Science, Royal Society of Chemistry
1998-2005	Co-organizer, placement program for (30+) students from the IUT system in France
2003-	Co-chair of the 7th International Conference on Calixarenes, Vancouver, B.C., Canada, 08/03
2004-	Ad hoc Reviewer, NIH General Medicine ZRG1 BCMB-M (10) B study section
2004-	Invited participant, NSF Young Investigator Supramolecular Chemistry Workshop
2006-	Ad hoc Reviewer, NIH, Synthetic and Biological Chemistry: A (SBC-A) Study Section
2007-	Invited participant, NSF Workshop on Complexity and Emergent Phenomena in Chemistry
2007-	Member for the NIH, Synthetic and Biological Chemistry: A (SBC-A) Study Section (2007-2011)
2009-2012	Associate Chair, Department of Chemistry, UNO, LA
2009-	Columnist, Nature Chemistry
2010-	Organizer, Supramolecular Chemistry Symposium, Joint SE/SW Regional ACS meeting, New Orleans
2011-	Member, International Advisory Committee, International Conference on Calixarenes
2013-	Co-Editor-in-Chief, *Supramolecular Chemistry* (Taylor and Francis Group)
2013-	Organizer and co-founder of the C. David Gutsche Award, a biennial $5000 award for senior researchers who have made a significant impact in the field of calixarene chemistry
2014-	Chair: Mardi Gras Symposium, Tulane University; a one-day symposium with 7 international speakers and 105 attendees (2014)
2015-	Visiting Professor, Wuhan University of Science and Technology as a Chair Professor of the Chutian Scholars Program (2015-2017)
2015-	Member, International Scientific Committee for the International Symposium on Macrocyclic and Supramolecular Chemistry (ISMSC) series
2015-	PI, NSF Workshop; “Accelerating our Understanding of Supramolecular Chemistry in Aqueous Solutions”
2015-	Consultant, Statistical Assessment of the Modeling of Proteins and Ligands (SAMPL), OpenEye Scientific

Honors and Awards:

1996	UNO Scholar Award
1998	Research Corporation, Research Innovation Award
1999	UNO Scholar Award
2001	UNO Science Research Development Award
2008-2011	UNO University Research Professor

C. Contributions to Science

The Hofmeister Effect. In large part because of improved molecular dynamics simulations and new surface-specific spectroscopic techniques, the last decade or so has seen a revival in the age-old problem of understanding the Hofmeister effect, i.e., the ubiquitous phenomenon whereby, irrespective of the physicochemical technique, ranges of salts are seen to influence the properties of water or aqueous solutions in predictable ways. As outlined in this application, our recent research with deep-cavity cavitands has affected science’s understanding of the Hofmeister effect by unequivocally demonstrating that even under unfavorable conditions, anions have a measurable and significant affinity for hydrophobic surfaces.[1-4] Furthermore, we have shown that anion binding influences the thermodynamics of (hydrophobic) guest binding to hosts in a manner that parallels the Hofmeister series.

From a personal perspective, understanding the Hofmeister effect is a large component of aqueous supramolecular chemistry. Yet the two groups of scientists who respectively study the Hofmeister effect and supramolecular chemistry in water have essentially remained separate. It is for this reason that our work has not only involved fundamental research at the boundary between these two fields, but has also involved efforts to bring these two fields together. This application – involving collaboration between a supramolecular chemist (the PI), a leader in molecular simulations and statistical thermodynamic theory of aqueous solutions (Ashbaugh), and an expert in hydration-shell vibration spectroscopic methods, densitometry, and theory (Ben-Amotz) – is one such local example of bringing these fields together. On a larger scale, the PI recently led a NSF supported workshop entitled, "*Accelerating our Understanding of Supramolecular Chemistry in Aqueous Solutions*". Held last May in Washington DC, this meeting brought together sixteen water scientists (physical chemists, computationalists, instrumentalists, physicists and biophysicists) and sixteen supramolecular chemists (physical-(in)organic chemists) to discuss each side's approach to solving mutual/related problems in the field. One metric of the success of this meeting was that an exit survey suggested twenty-four new collaborations between pairs of attendees in the two fields. Further such endeavors are ongoing.

1) Sokkalingam P., Shraberg J., Rick S. W., Gibb B. C. Binding Hydrated Anions with Hydrophobic Pockets. *J. Am. Chem. Soc*., **2016**, *138*(1), 48-51.
2) Gibb C. L. D., Oertling E. E., Velaga S., Gibb B. C. *Thermodynamic Profiles of Salt Effects on a Host-Guest System: New Insight into the Hofmeister Effect*. Journal of Physical Chemistry B, **2015**, *119*(17), 5624-38
3) Carnagie R., Gibb C. L. D., Gibb B. C. *Anion Complexation and The Hofmeister Effect*. Angew. Chem. Int. Ed., **2014**, *53*(43), 11498-500
4) Gibb C. L. D., Gibb B. C. *Anion binding to hydrophobic concavity is central to the salting-in effects of Hofmeister chaotropes*. J. Am. Chem. Soc., **2011**, *133*(19), 7344-7

Assemblies driven by the Hydrophobic Effect. With the exception of cyclodextrin chemistry, which had mostly peeled away from supramolecular chemistry and moved decidedly into a more applied realm, when I began my independent career, supramolecular chemistry was primarily studied in organic solvents. State-of-the-art in regards to self-assembled hosts/supramolecular containers were the (hydrogen bonded) Rebek "jelly doughnut" and (metal coordinated) L_4M_6 cages from the Fujita lab. My goal was to work in water, and I wanted to avoid these two common strategies for assembly – hydrogen-bonding and metal coordination – and use the Hydrophobic effect to drive the formation of structurally specific, mono-dispersed supramolecular containers large enough to encapsulate sizable guests. We first designed and synthesized more straightforward hosts soluble in organic solvents, before devising the first host that relied solely on the Hydrophobic effect to drive assembly.[1] This deep-cavity cavitand, as well as related hosts we have synthesized, define a dry, yocto-liter sized environment by dimerizing around guest molecules. Their ease of synthesis, combined with their encapsulation properties, is reflected in the fact that at least six laboratories around the world have independently worked with these types of hosts.[1] Since that time, others have entered this new field with their own self-assembling systems; most notably Mitsuhiko Shionoya (U. Tokyo) and Michito Yoshizawa (Tokyo Institute of Technology). Our research has now expanded to include the formation of tetrameric and hexameric assemblies that represent the largest such structures devised to date.[2,3] *En masse*, these supramolecular containers have provided valuable information about the structural requirements for controlled assembly using the Hydrophobic effect, and in conjunction with the concomitantly developing cucurbiturils, are shedding light on how the Hydrophobic effect can be orchestrated to control supramolecular properties.[4]

1) Jordan, J. H., Gibb, B. C., Molecular containers assembled through the hydrophobic effect, *Chem. Soc. Rev.,* **2015,** *44* (2), 547-85
2) G Gan H., Benjamin C. J., Gibb B. C. *Non-monotonic Assembly of a Deep-Cavity Cavitand*. J. Am. Chem. Soc., **2011**, *133*, 4770-3
3) Gan H., Gibb B. C. *Guest-Mediated Switching of the Assembly State of a Water-Soluble Deep-Cavity Cavitand* Chemical Communications, **2012**, *49*, 1395-7.
4) Hillyer M. B., Gibb B. C. *Molecular Shape and the Hydrophobic Effect*. *Annu. Rev. Phys. Chem*., **2016**, *67*, 307-29.

Controlling Photochemistry and Photophysics. In collaboration with V. Ramamurthy (U. Miami) we have advanced the ability to control photochemical and photophysical processes in aqueous solutions.[1-4] Our self-assembling containers have opened up the range of processes that can be studied in water, and brought a new level of control in regards to not only cage-effects, but also to the regioselectivity and stereoselectivity of these processes. In short, we have demonstrated that the hydrophobic effect can be orchestrated to bring about selective complexation and assembly so as to force photochemical and photophysical processes down pathways that do not exist in free solution (or even in structurally defined media such as zeolites). Furthermore, our work demonstrated for the first time cross-talk between supramolecular complexes that mimic chemical signaling between enzymes.[3]

1) Kaanumalle L. S., Gibb C. L. D., Gibb B. C., Ramamurthy V. *Controlling Photochemistry with Distinct Hydrophobic Nano-Environments*. *J. Am. Chem. Soc*., **2004**, *126*, 14366-7
2) Kaanumalle L. S., Gibb C. L. D., Gibb B. C., Ramamurthy V. *A Hydrophobic Nano-Capsule Controls the Photophysics of Aromatic Molecules by Suppressing their Favored Solution Pathways*. *J. Am. Chem. Soc.*, **2005**, *127*, 3674-5.
3) Natarajan A., Kaanumalle L. S., Jockusch S., Gibb C. L. D., Gibb B. C., Turro N. J., et al. *Controlling Photoreactions with Restricted Spaces and Weak Intermolecular Forces: Remarkable Product Selectivity during Oxidation of Olefins by Singlet Oxygen*. *J. Am. Chem. Soc.*, **2007**, *129*, 4132-3. See also commentary: Greer A. *Molecular Cross-Talk*. Nature, **2007**, *447*, 273-4.
4) Gibb, C. L. D.; Sundaresan, A. K.; Ramamurthy, V.; Gibb, B. C., Templation of the Excited-State chemistry of α-(n-Alkyl) Dibenzyl Ketones: How guest packing with a nano-scale supramolecular capsule influences photochemistry. *J. Am. Chem. Soc.* **2008,** *130*, 4069-4080

Molecular Protections and Separations. The supramolecular systems devised in the group have many unusual and unique properties resulting from their ability to engender compartmentalization. One area that we have helped pioneer, and an area that is very much ongoing in our lab, is to use these nano-containers as a means to bring about molecular separations. Although these processes can be made more complex by the binding of two different guests within a container,[1] we have reported on a number of different approaches. One example is the physical separation/purification of hydrocarbon gases using aqueous solutions.[2] Thus, when a mixture of, for example, propane and butane is added to the head space above a solution of one of our water-soluble hosts, it is observed that only butane is pulled into solution (to form the corresponding 2:2 host-guest complex), leaving behind an enriched/pure sample of propane in the gas-phase. Such purifications are beyond the state-of-the-art of semi-permeable membrane technology. We have also demonstrated how molecular containers can be use to bring about chemical separations of normally difficult-to-separate mixtures.[3] One example of such kinetic resolutions is to add a mixture of two guests to a hydrolytic solution containing a host. The guest that binds preferentially is protected within the nano-container, whilst the less complementary guest is exposed to the reactive solution and hydrolyzed. This type of kinetic resolution via molecular protection represents a new strategy for separating complex mixtures.

1) Sullivan M. R., Gibb B. C. *Differentiation of small alkane and alkyl halide constitutional isomers via encapsulation*. Special issue on aqueous supramolecular chemistry, Org. Biomol. Chem., **2015**, *13*(6), 1869-77
2) Gibb C. L. D., Gibb B. C. *Templated Assembly of Water-Soluble Nano-Capsules: Inter-Phase Sequestration, Storage, and Separation of Hydrocarbon Gases*. *J. Am. Chem. Soc*., **2006**, *128*(51), 16498-9
3) Liu, S.; Gan, H.; Hermann, A. T.; Rick, S. W.; Gibb, B. C., Kinetic Resolution of Constitutional Isomers Controlled by Selective Protection inside a Supramolecular Nanocapsule. *Nature Chemistry* **2010,** *2* (10), 847-852

Editorship. As co-editor in chief of *Supramolecular Chemistry* (along with Philip Gale, U. of Southampton) I am fortunate to be in a position to help shape the future of the field. Although relatively specialized, the journal provides a valuable forum for countless authors from both developed nations and newly industrialized countries such as China and India. Moreover, the journal works closely with a number of international conferences including: the International Symposium on Macrocyclic and Supramolecular Chemistry, the International Conference on Molecular Sensors and Molecular Logic Gates, the International Conference on Calixarenes, and the International Conference on Cucurbiturils. Through these collaborations the journal helps support these meetings and produces special issues dedicated to each conference. Relatedly, the journal also publishes thematic special editions on a range of subjects, as well as those dedicated to honoring leaders in the field. In addition, we also publish invited "big picture" essays from world leaders on their opinions of the state-of-the-art and future of the field. In combination, these different activities mean that *Supramolecular Chemistry* is not only a key forum for everything supramolecular, but that it also helps glue, shape and direct the field.

Complete list of Published Work: http://www.gibbgroup.org/blog/wp-content/uploads/2013/08/Gibb-CV.pdf

D. Research Support

NIH R01 GM098141 Gibb (PI) 06/01/12-02/28/17
Using Deep-Cavity Cavitands to Study Supramolecular Chemistry in Water
The goal of this study is to contribute to our understanding of the Hofmeister Effect by probing how anions influence binding events driven by the Hydrophobic effect.
Role: PI

NSF CHE 1450865 Gibb (PI) 02/15/15-01/31/17
Accelerating our Understanding of Supramolecular Chemistry in Aqueous Solutions: A Workshop Proposal
The goal of this study was to organize a workshop to bring together two separate groups of scientists: water and aqueous solutions scientists, and supramolecular chemists.
Role: PI

NSF CHE 1507344 Gibb (PI) 08/15/15-08/14/18
Nano-Containers for Novel Separations and Reactions
The goal of this study is to investigate self-assembled dimeric nano-capsules as yocto-liter reaction flasks and as containers for the separation of complex mixtures of small (< C20) molecules.
Role: PI

NSF CBET 1403167 Ashbaugh (PI) 07/01/14-06/30/17
Capacious Deep-Cavity Cavitand/Hydrophobic Guest Assemblies with Tunable Interior Volumes
The goal of this grant is to understand how hydrophobe shape influences the Hydrophobic effect and how this in turns influences the formation of self-assembled supramolecular containers.
Role: co-PI

NSF 143280 Khonsari (PI) 08/01/14-07/31/17
The Smart MATerial Design, Analysis, and Processing (SMATDAP) consortium: Building next-generation polymers and the tools to accelerate cost-effective commercial production
The goals of this award are to develop new, real-time and multi-channel analysis of polymerization processes, particularly in regard to the development of supramolecular polymers.
Role: co-PI

Completed Research Support
NIH 1S10OD020117-01 Jayawickramarajah (PI) 03/09/15-03/08/16
Acquisition of a Surface Plasmon Resonance Biosensor: Enhancing Biomedical (Bio)Molecular Recognition Projects
This was an equipment award for the purchase of a new Surface Plasmon Resonance.
Role: co-PI

Louisiana Board of Regents (LEQSF(2015-16)-ENH-TR-39 Grayson (PI) 03/09/15-03/08/16
Nano-materials Separation and Characterization Equipment
This was an award for the purchase of new GPC equipment.
Role: co-PI

NSF CHE 1244024 Gibb (PI) 05/31/12-07/31/15
Studies of Deep Cavity Cavitands
The goals of this award were to: devise multi-(supra)molecule systems possessing unusual relationships between the components, the environment and the net overall state of the system, and study encapsulation approaches to the separation of constitutional isomers.
Role: PI

NSF CHE 1228232 Mague (PI) 09/01/12-08/31/15
MRI: Acquisition of a Single-Crystal, Micro-Source Diffractometer
This was an award for the purchase of new diffractometer.
Role: co-PI